NUMERICAL SIMULATION & MODELING OF THIN-FILM HETEROJUNCTION PHOTOVOLTAIC CELLS AND ITS DEGRADATION ANALYSIS

Synopsis

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KHUSHBOO DIXIT

Under the supervision of

DR. GUFRAN AHMAD
(Assistant Professor)
DEPARTMENT OF ELECTRICAL ENGINEERING
FACULTY OF ENGINEERING

DEPARTMENT OF ELECTRICAL ENGINEERING

FACULTY OF ENGINEERING

DAYALBAGH EDUCATIONAL INSTITUTE

DAYALBAGH, AGRA-282005

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1. Introduction

1.1 Solar cell: - The photovoltaic cell or solar cell is an electronic device, which converts solar radiation into electrical energy. The working principle of solar cell is "photovoltaic effect". When solar radiation falls on solar cell it performs two major operation: generation of photo generated charge carrier (holes and electrons) in absorption layer and separation and collection of these charge carrier at their respective metal contacts. Operation of solar cells are divided in four major steps:-

i. Generation of photo generated carriers (electrons and holes)

ii. Collection of photo generated carriers (current generation)

iii. Generation of a large voltage across the solar cell.

iv. Power dissipation at the load.

In solar cell, semiconductor layers are the most important part because the subsequent separation of the photo-generated charge carriers take place in it. There are a number of different semiconductor materials that are suitable for the conversion of energy of photons into electrical energy. The crystalline silicon solar cell due to its simple structure dominated the photo voltaic market for many years.

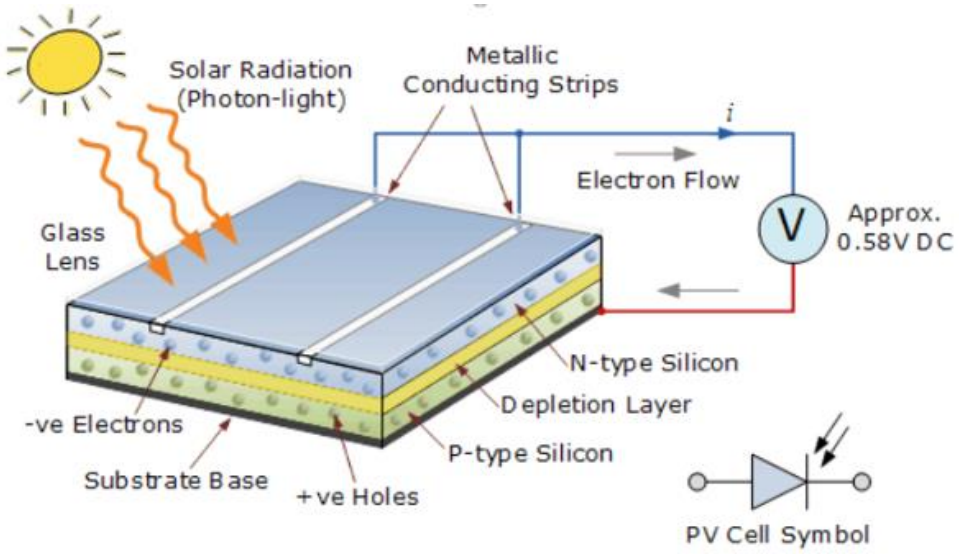

Figure 1: Typical Silicon based solar cell
(Source: https://electricalengineering123.com/solar-cell-construction-working-principle/)

yAn absorber material is a moderately doped p-type square wafer having thickness of 300 µm and an area of 10 × 10 cm^2 or 12.5 × 12.5 cm^2. On both sides of the c-Si wafer a highly doped layer is formed, ($n+$ type on the top side and $p+$ type on the back side) these doped layers help to separate the photo-

generated charge carriers from the bulk of the c-Si wafer. Both sides of solar cell consist of a top and bottom metallic grid or electrical contact that collects the separated charge carriers and flow it through the external circuit by using these front and back metal contacts. Usually, a thin layer called antireflective coating covers the topside of the cell in order to decrease the reflection of light from the cell. A glass sheet or other type of transparent encapsulant is attached to both sides of the cell in order to protect the cell against the effects of outer environment during its operation. When the processing temperature during the deposition of the layers is low, a wide range of low-cost substrates such as metal, glass sheet or polymer foil can be used. The semiconductor parameters that determine the design and performance of a solar cell are:-

i) Concentrations of doping atoms to determine the width of a space-charge junction.

ii) Mobility (μ) and diffusion coefficient (D) of charge carriers that characterize carriers transport due to drift and diffusion, respectively.

iii) Lifetime (τ) and diffusion length (L) of the excess carriers that characterize the recombination-generation processes.

iv) Band gap energy (E_g), absorption coefficient (α) and refractive index (n) that characterize Ability of a semiconductor to absorb visible and other radiation.

1.2 Photovoltaic effect: - Photovoltaic effect is a phenomenon which convert electromagnetic light radiation directly into electrical energy. Solar cell is a device used for the conversion of sunlight into usable electrical energy. Sunlight is an input source in the photovoltaic cells, It transforms sunlight into electricity. When sunlight falls on the photovoltaic cell then electrons moves freely in semiconductor material. If wires are connected to the positive and negative terminals of a photovoltaic cell, electron started to flow and electricity is produced. This electricity is further used to power an electric load. [23]

1.3. Working principle of photovoltaic cell: -Photovoltaic cell works on the principle of photovoltaic effect. This effect results in the formation of a potential difference due to electromagnetic at the junction of two different materials. The photovoltaic effect can be divided into the following three basic processes. [24].

1.3.1 Generation of charge carriers due to photon absorption:- Photon absorption in photovoltaic material excites the electrons and they move from initial energy state Ei to higher energy state E_f as

given in Figure 2(a). It shows that photon energy $Eph = hv$ excites electrons present in the valence band (E_i, initial energy state) shifted to the conduction band (E_f, final energy state) after absorption of photon energy. Figure 2(b) shows that if $Eph > Eg$, a part of the energy is thermalized. Photon energy can be absorbed in the presence of Ef and Ei electron energy levels. Photon energy is equal to the difference of Ef and Ei as given in equation.

$$hv = E_f - E_i \quad (1)$$

In ideal case electron populates below then valence band edge Ev and above the edge of conduction band Ec in semiconductor. There is no other energy level for the electron population in amongst these two states. Hence the energy difference between Ec and Ev is called the band gap energy. Therefore, the photon energy smaller than this band gap energy will not be absorbed.

$$E_g = E_c - E_v \quad (2)$$

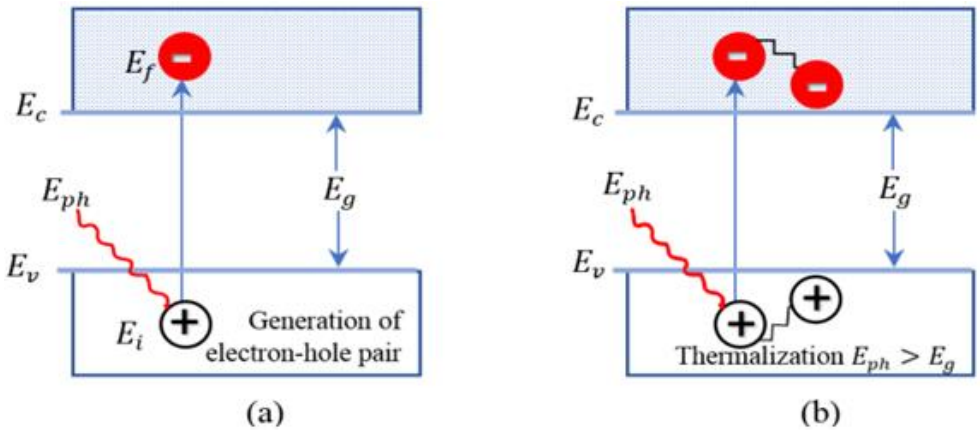

Figure 2: Generation of charge carriers by photon absorption (https://www.researchgate.net/publication/332736236_Modeling_of_High_Power_Conversion_Efficiency_Thin_Film_Solar_Cells).

1.3.2 Recombination of charge carriers: - The electron will fall back to its initial energy state and releases energy in a form non- radiative recombination (transfer of energy to other holes and electrons) or radiative recombination (photon emission). The semi membrane presence on both sides of the absorber allows the use of energy stored in these electron-hole pairs in an external circuit. Electrons and holes are separated due to semipermeable membranes electron flows out from one membrane whereas holes flows from other membrane. P-type and n-type materials are used for membrane formation. The solar cell is designed in such a way that before recombination of electron-hole pair, they must be reached

to the membrane. It means that the time required to reach these charge carriers to their respected membrane must be shorter than their lifetime, due to this absorber thickness is limited.

1.3.3 Extraction of photogenerated charge carriers: - After light absorption photo-generated charge carrier is extracted by using externally connected electrical contacts and allows the energy use in the external circuit. In this stage, light energy is converted into electrical energy. At the back contact and absorber layer, electrons recombine with holes after passing from the external circuit.

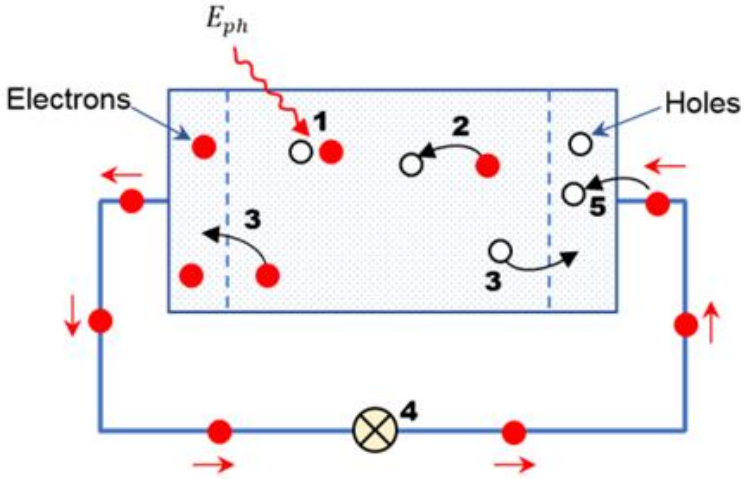

Figure 3: Extraction of photo-generated charge carriers
(Source:https://www.researchgate.net/publication/332736236_Modeling_of_High_Power_Conversion_Efficiency_Thin_Film_Solar_Cells)

1.4 V-I characteristic of a photovoltaic device: - V-I characteristics curve is the graphical representation of the operation of a photovoltaic cell. It can be well understood by considering the equivalent circuit of a solar cell. *V-I* characteristic of a photovoltaic cell is the superposition of the *V-I* curve of a device in dark (absence of light) and illuminating (under light) conditions [28, 29]. In dark conditions photovoltaic cell has similar electrical characteristics as of large diode. When light falls on the photovoltaic cell, electrical power can be extracted and VI curve down into the fourth quadrant. Amount of shift is directly proportional to the incident light intensity on a solar cell as shown in Figure 4. Where maximum power is indicated by the shaded area. Illuminated cell added with diode dark currents, diode law becomes:

$$I = I_0 \left[exp\left(\frac{qv}{\mathrm{nkT}}\right) - 1\right] - I_L \qquad (3)$$

Where I_0 = diode leakage current under dark or dark saturation current, I_L= light generated current, V= applied terminal voltage across diode, q = electronic charge, k= Boltzmann's constant n = Ideality factor and T= temperature.

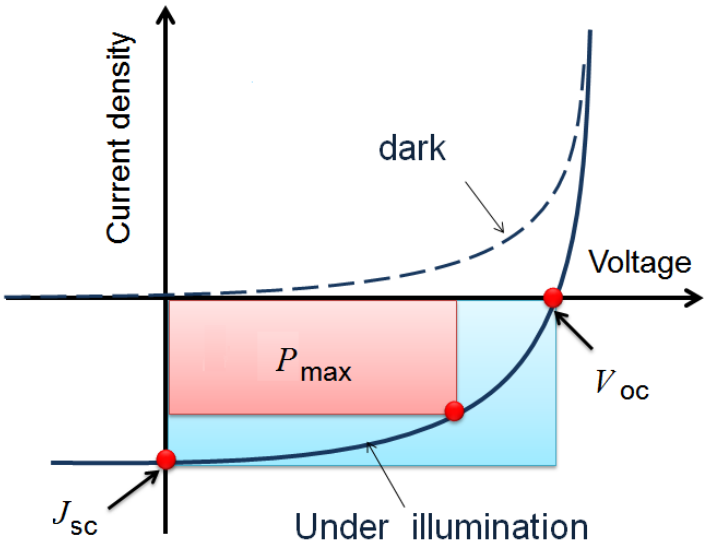

Figure 4: V-I characteristic of photovoltaic cell under illuminated and dark (Source:https://www.researchgate.net/publication/332736236_Modeling_of_High_Power_Conversio_Efficiency_Thin_Film_Solar_Cells).

1.5 Generations of solar cells: -Traditionally solar cells are divided into three generations.

1.5.1 First generation solar cells: - First generation ($1G$) of solar cells is mainly based on silicon wafers and typically the power conversion is about 15-20% [18]. Generally, in comparison of non-silicon based solar cells, this solar cell technology is more efficient and of longer life but at the higher temperature, they are more peril to lose some part of their efficiency. Currently, four types of silicon-based photovoltaic cells are commercially used for the manufacturing of solar panels. These types are monocrystalline, polycrystalline, amorphous and hybrid solar cells.

1.5.2 Second Generation solar cells:- Second generation ($2G$) of solar cells are based on amorphous silicon and non-silicon materials namely copper indium gallium selenide ($CIGS$) and cadmium telluride ($CdTe$), where typically the power conversion efficiency is about 10-15% [6]. Use of silicon wafers are avoided in second generation solar cell and consumption of lower material reduces the production cost of $2G$ solar cells in comparison of the first-generation solar cell. This cell generation class is also known as thin film solar cells because of using only few micrometre thicknesses of different layer materials in comparison of crystalline silicon based cells. This type of technology is commercially using because of

lower manufacturing cost and using less material. The second-generation solar cells production is still limited due to the use of rare elements and high-temperature treatments. So, the production cost is less than the first generation solar cell but still higher than other technologies.

1.5.3 Third Generation solar cells:- In this new technology solar cells are made from the variety of new materials rather than using silicon such as solar inks using in printing technology, silicon wires, nanotubes, conductive plastics, and organic materials. The goal is to improve the commercially available solar cell by enhancing the efficiency and to reduce the cost to make them economical. Currently new class of thin film solar cells. Under investigations are perovskite solar cells and quaternary compounds material based solar cells such as kesterite solar cells. These types of devices show an enormous potential with record power conversion efficiency of about 20% on a very small area [17]. In the comparison of first and second-generation solar cells, third generation solar cells are limited but they have great potential. Recently research interest is significantly increases in polymer solar cells. [43].

1.6 Different types of solar cells:-Solar cells are divided into two major groups. They are silicon semiconductor type and non-silicon type. The details are as follows.

1.6.1 Monocrystalline solar cell: - These types of solar cells belong from first-generation solar cell technologies. The width of the wafer used in these types of solar cells is up to 200μm. The cell slice is cut from a pure silicon bar, which allows them to more efficiently converting the sunlight radiation energy into electrical energy. The complete cell is aligned in the same direction, so when the light falls on the cells at the accurate direction, they are very efficient. In a sunny day, photovoltaic cells work best with the sunlight directly falls on accurate direction. They are absorbing most of the solar radiation, so they have a uniform blacker colour. Cost of the production of these types of solar cells is more than in the comparison of a polycrystalline cell. In a comparison of polycrystalline, monocrystalline is the most efficient type of photovoltaic solar cells.

1.6.2 Polycrystalline solar cell: - These types of solar cells also belong from first-generation solar cell technologies. These cells are made up of several silicon cells joined together instead of using a single crystal of silicon. In general, the cost of production of a polycrystalline solar cell is not much higher than monocrystalline. Therefore, they are also more affordable. In comparison with a monocrystalline

solar cell, the power conversion efficiency of polycrystalline solar cell is less. Their overall manufacturing design can often make up for the efficiency loss.

1.6.3 Amorphous solar cell: - Amorphous silicon (a - Si) solar cells belong from a thin-film solar cell. In these types of solar cells, one or more layers of photovoltaic materials are deposit on a substrate. In comparison with other technologies, they have low manufacturing cost. To make thin-film photovoltaic solar cells, manufacturers spray a layer of silicon on a substrate. They are produced by placing one or more thin layers of photovoltaic composite on a substrate. Thin film photovoltaic solar cells are different from other types; they are also more flexible than other types. It can be put onto different surfaces i.e. curved and straight.

1.6.4 Other types of solar cell: - Silicon-based solar cells are most commonly used solar cells. There are some other types such as ($CIGS$) and cadmium telluride ($CdTe$) based solar cells, kesterite and perovskite solar cells, which are also used due to their good conversion capabilities, earth-abundant materials, and enhanced power conversion efficiencies.

1.6.5 Thin film solar cells: - Thin film photovoltaic solar cells belong from second and third generation solar cell technology. These types of solar cells are manufactured by depositing one or more layers of photovoltaic materials on a metal, plastic or glass substrate. Commercially thin film photovoltaic solar cells are used in various technologies, such as copper indium gallium selenide ($CIGS$), cadmium telluride ($CdTe$), kesterite and perovskite solar cell technologies. The film thickness of these types of solar cells varies from few nm to tens of μm due to this, these types of solar cells are flexible and lower in weight. Thin film technology is cheaper than other technologies because of devices have relatively less material. Thin film photovoltaic technologies are based on various types of light absorbers semiconductor materials. The absorption coefficient of these types of materials is higher than crystalline materials. Therefore, a very thin layer of the absorber layer is sufficient for the effective absorption of sunlight. Historically in the thin film technology, amorphous silicon-based solar cells played a momentous role.

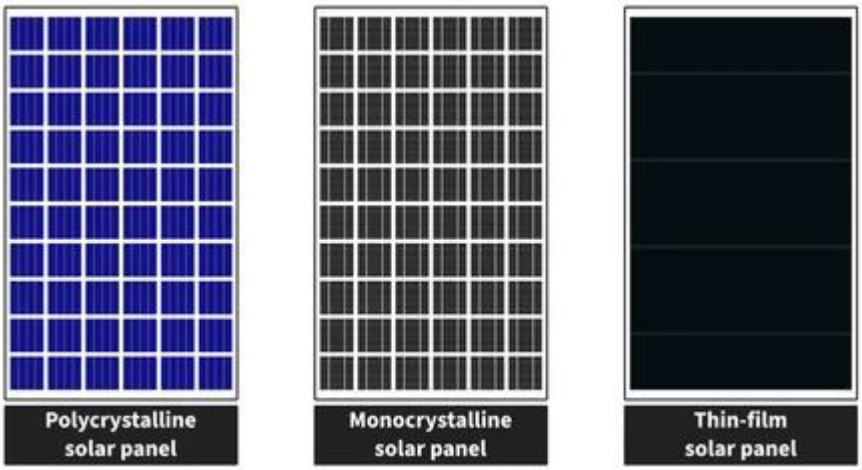

Figure 5: Types of photovoltaic solar cells
(Source: https://www.shutterstock.com/image-vector/different-types-solar-panels-polycrystalline-monocrystalline-1964242153)

1.7 Basic parameters of solar cells

1.7.1 Short circuit current: - The maximum current flow through the solar cell at zero load condition (at $RL = 0$) or short-circuited is known as short-circuit current (Isc). At the largest value of Isc, the voltage of a solar cell will be zero [26]. The flow of Isc is due to the collection and generation of light generated carriers. It mainly depends on the number of incident photons as well as the spectrum, area of solar cell, optical properties and the collection probability of light generated carriers.

1.7.2 Open circuit voltage:- The maximum voltage is taken from the solar cell (at $R_L = \infty$) is known as open circuit voltage (V_{oc}). When a solar cell is an open circuited, and no load is connected across the solar cell then current will be at its minimum (zero) value whereas the voltage will be at maximum value [12]. From solar cell equation, V_{oc} can be derived by setting net current to zero and is given in equation 4.

$$\mathrm{Voc} = \frac{nkT}{q} \ln\left(\frac{\mathrm{IL}}{\mathrm{I0}} + 1\right) at\ I = 0 \qquad (4)$$

From the above equation, it is clear that open circuit voltage depends on I_0 (saturation current) and I_L (light generated current). I_0 depends on recombination in the solar cell. So, V_{oc} is a measure of the amount of recombination in a solar cell.

1.7.3. Fill factor: - The measure of a photovoltaic cell quality is fill factor (FF), which is derived by equating the maximum power (P_{max}) to the theoretical power (P_t). Where power (P_t) would be output

at both the open circuit voltage (V_{oc}) and short-circuit current (J_{sc}) as given in equations 5 & 6 [30]. Fill factor can be interpreted graphically as the ratio of the rectangular areas.

$$FF = \frac{Pmax}{Pt} \tag{5}$$

$$FF = \frac{Vmax\ .Imax}{Voc\ .Isc} \tag{6}$$

1.7.4. Maximum power: - The output power of a solar cell is given in watts and is equal to the product of voltage times the current and is defined as

$$P_{\text{out}} = P_{\text{out}}\ \text{I}_{\text{out}} \tag{7}$$

Under short and open circuit conditions, no power is generated. The power output will be zero if both or anyone will be zero. The device will provide maximum power for maximum values of voltage and current.

$$P_{\text{max}} = P_{\text{max}}\ \text{I}_{\text{max}} \tag{8}$$

By putting Equation 6 in Equation 8 we get,

$$P_{\text{max}} = \text{V}_{\text{oc}}\ \text{I}_{\text{sc}}\ \text{FF} \quad \textit{(In terms of FF)} \tag{9}$$

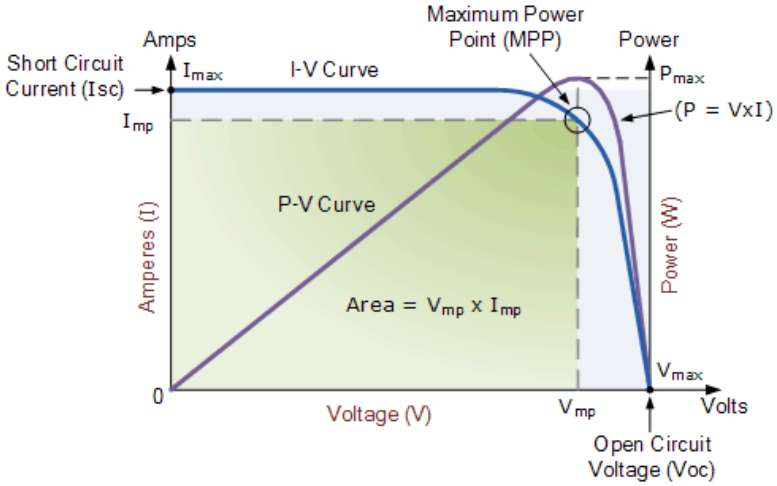

Figure 6: Attaining fill factor from VI characteristics curve
(Source: https://electronics.stackexchange.com/questions/619252/determine-voltage-and-current-for-given-i-v-curve)

1.7.5. Power conversion efficiency: - Power conversion efficiency is the most frequently used parameter to relate the performance of two solar cells and is termed as PCE. It is defined as the ratio of

output power from a solar cell to the input power from the sun [12].

$$PCE = \frac{\text{Pmax}}{\text{Pin}} \quad (10)$$

$$P_{\text{max}} = \text{v}_{\text{oc}}\, \text{I}_{\text{sc}}\, FF \quad (11)$$

$$P_{\text{t}} = \text{v}_{\text{oc}}\, \text{I}_{\text{sc}} \quad (12)$$

Therefore, from equation 10 and 11 the product of theoretical power (Pt) and fill factor (FF), divided by power the energy input from the sun is the power conversion efficiency [31]. Mathematically expressed in equation 13.

$$PCE = \frac{\text{voc Isc FF}}{\text{Pin}} \quad (13)$$

PCE depends on the parameters like incident sunlight intensity, solar cell working temperature and spectrum type. So, to compare two or more solar cells, it is important to carefully control the conditions under which PCE is measured.

1.7.6. Quantum efficiency: - The quantum efficiency (QE) is the ratio of the extracted free charge carriers by the solar cell to the number of incident photons. In other words, QE relates to the response of a solar cell to different wavelengths. It may be given either as a function of energy or wavelength. The QE will be unity at the precise wavelength if all certain wavelength photons are absorbed and the resulting minority carriers are collected.

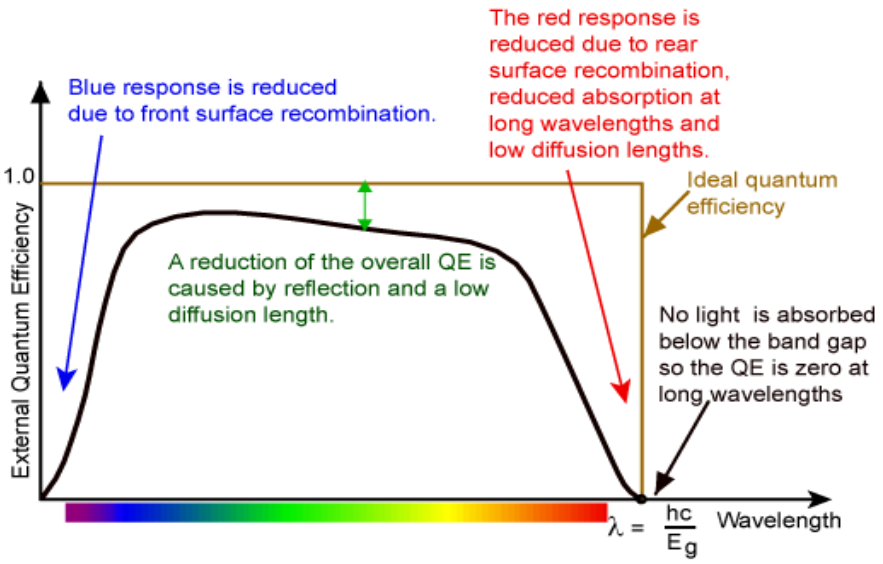
The red response is reduced due to rear surface recombination, reduced absorption at long wavelengths and low diffusion lengths.
Blue response is reduced due to front surface recombination.
1.0
External Quantum Efficiency
Ideal quantum efficiency
A reduction of the overall QE is caused by reflection and a low diffusion length.
No light is absorbed below the band gap so the QE is zero at long wavelengths
λ = hc/Eg
Wavelength

Figure 7: Quantum efficiency curve
(Source: https://www.pveducation.org/pvcdrom/solar-cell-operation/quantum-efficiency)

2. Review of literature

American Physical Society explains the history of a solar cell in its publication "APS News" volume 18, issue 4 in April 2009 [40]. According to APS news antiquity of solar cell is based on French physicist Alexandre-Edmond Becquerel observations of the photovoltaic effect in 1839 but he couldn't explain that effect. In 1873 English engineer named Willoughby Smith discovered the photoconductivity of selenium. Charles Fritts was an American inventor and in 1883 he designed the first selenium based solar cells but the efficiency of a cell was less than 1% to convert the sunlight energy to electrical energy. So, this design was not very. The next major advancement in solar cell technology was made in 1940 by Russell Shoemaker Ohl, a semiconductor researcher at Bell Laboratories he made a p-n junction based solar cell. Ohl patented his solar cell and the conversion efficiency was about 1%. After thirteen years, the first silicon-based practical solar cell was made by scientist's team working at Bell Labs. They were facing two issues in their work first issue was producing good electrical contacts; the other problem was that over time lithium migrated through the silicon at room temperature and moves away from sunlight. To solve these problems they tried different impurities, finally arsenic and boron were selected these elements created p-n junction stayed close to surface, also they found that with boron-arsenic and silicon cells they can make good electrical contacts. One of the attractive features of α-Si is that it is a direct band gap material, which allows a significant fraction of sunlight to be absorbed within a thin layer of a few micrometers [1]. However, short orders in amorphous material and the dangling bonds result in short minority carrier diffusion lengths and abnormal electrical behaviour [6]. Hydrogen passivation, also designated as α-Si: H, can reduce dangling bond densities by several orders of magnitude, thus helping to improve the minority carrier length. However, this hydrogenation is responsible for the Staebler-Wronski light degradation effect this leads to the development of thin film solar cells. Now a day's researcher's move towards cadmium telluride ($CdTe$) and copper indium gallium selenide ($CIGS$) based thin film devices because of their high efficiency and good performance and reached in the commercial stage. In research and development scale these technologies have power conversion efficiency up to 21.37 % [3] while commercially they have a conversion efficiency of 17-18 % [45, 46]. The photovoltaic performance (efficiency η) of an ITO/CdS/CdTe structure cell is studied by Seck, Serigne Massamba, et al. The

study is carried out by simulation with SCAPS (Solar Cell Capacitance Simulator) whose mathematical model is based on solving the equations of Poisson and continuity of electrons and holes. An electrical conversion efficiency of 23.58% is obtained by optimizing the mobility of the electrons (100 cm^2 /Vs), that of the holes (25 cm^2 /Vs), the density of electrons (10^{15} cm^{-3}), the density of the effective states in the conduction band (7.9×10^{17} cm^{-3}) and the electronic affinity (3.85 eV) of the CdTe absorbent layer [1,3]. Messmer, Christoph, et al in their study proved that Transition metal oxides (TMOs) are of increasing importance for many applications reaching from thin-film transistors and non-volatile memory to novel contact layers in photovoltaic. Due to their tunable electrical properties and high transparency, TMOs are also promising candidates as contact layers in silicon heterojunction solar cells already leading to cell efficiencies of about 22% [7,11].For the fabrication and development of low cost and sustainable thin film photovoltaic cells kesterite based absorber materials are intensively studies such as copper zinc tin sulfide $Cu2ZnSnS4(CZTS)$, Copper zinc tin selenide $Cu2ZnSnSe4(CZTSe)$ and sulfur-selenium alloy $Cu2ZnSn(SxSe1\text{-}x)4$ $(CZTSSe)$ [47– 53]. These materials drawing attention because of their good optical properties for photovoltaic applications [54]. These absorber materials are copper based nontoxic semiconductor materials [55]. They are the good replacement for the chalcopyrite absorbers by replacing indium (In) with comparatively inexpensive zinc (Zn) and gallium (Ga) with tin (Sn) in the $CIGS$ absorbers [6–8]. The outstanding features and efficient performance of these kesterite based materials made them very fascinating in the thin film's community [56, 57].

3. Methodology

3.1 Numerical modelling: - Numerical modeling is a computer simulation program which uses the mathematical equation for the implementation of a physical system. Numerical modeling is the tool to study the system behaviour and helps provide analytical solutions. Numerical analysis can play a significant role in the manufacturing and fabrication of efficiently working semiconductors based photovoltaic devices. For design engineers and researchers, the highest priority job of numerical modeling techniques implementation is the integration of real-life problem with virtual machine environment because of finding the optimum and efficient ways for solving a complex problem. The precious time is saved due to performing the real design problem in computer-based tests environments without physical or practical implementation, so research institutions and universities emphasize

computer-based learnings techniques. The modeling techniques are used to compute the fundamental physical properties such as holes and electrons concentration and electrical potential. It also provides more information regarding the influence of material physical parameters on device functional parameters or characteristics. For the numerical modeling of solar cells, physical parameters of material are taken as input for the simulation software. To translate the practical or real device *J - V* characteristics and functional parameters such as power conversion efficiency, fill factor, open circuit voltage and short circuit current in device modeling, it is mandatory to take experimental data. Numerical simulation provides a better and easier way to understand the device behavior. For the better understanding of the performance of a device, the simulation software that can be used for device modelling must be able to solve semiconductor basic equations like continuity equation for holes and electrons and the Poisson equation relating the charge to electrostatic potential.

3.2 Basic semiconductor governing equation:-

3.2.1 Continuity Equations: Drift, diffusion, and recombination-generation processes give rise to a change in the carrier concentrations in time. Nevertheless, there must be a spatial and time continuity in the carrier concentrations. The combined effect of all types of carrier action within a semiconductor is described by the following continuity equation for electrons (Eq. 14) and holes (Eq. 15) respectively.

$$\frac{\partial n}{\partial t} = \frac{\partial n}{\partial t}\Big|_{drift} + \frac{\partial n}{\partial t}\Big|_{diff} + \frac{\partial n}{\partial t}\Big|_{thermal\ R-G} + \frac{\partial n}{\partial t}\Big|_{other\ processes(photogeneration)} \quad (14)$$

$$\frac{\partial p}{\partial t} = \frac{\partial p}{\partial t}\Big|_{drift} + \frac{\partial p}{\partial t}\Big|_{diff} + \frac{\partial p}{\partial t}\Big|_{thermal\ R-G} + \frac{\partial p}{\partial t}\Big|_{other\ processes(photogeneration)}$$

The continuity equations can be written in a more compact form when introducing below substitutions

$$\frac{\partial n}{\partial t}\Big|_{thermal\ R-G} = -Rn \quad (16)$$

$$\frac{\partial p}{\partial t}\Big|_{thermal\ R-G} = -Rp \quad (17)$$

$$\frac{\partial n}{\partial t}\Big|_{other\ process} = -G \quad (18)$$

$$\frac{\partial p}{\partial t}\Big|_{other\ process} = -Gp \quad (19)$$

And noting down (Eq. 20) & (Eq. 21)

$$\frac{\partial n}{\partial t}\Big|_{drift} + \frac{\partial n}{\partial t}\Big|_{diff} = \frac{1}{q}\Delta \text{ Jn} \quad (20)$$

$$\frac{\partial p}{\partial t}\ \Big|_{drift} + \frac{\partial p}{\partial t}\ \Big|_{diff} = \frac{-1}{q}\Delta \text{ Jp} \tag{21}$$

In these equations $\partial n/\partial t$ ($\partial p/\partial t$) is the time rate change in the electron (hole) concentration, $\boldsymbol{J_n}(\boldsymbol{J_p})$ is the electron (hole) current density, $\boldsymbol{R_n}(\boldsymbol{R_P})$ denotes the net recombination-generation rate of electrons (holes), $\boldsymbol{G_n}(\boldsymbol{G_P})$ is the generation rate of electrons (holes) due to other processes, such as photo generation. By substituting equation 16, 17, 18 & 19 into equation 14 &15 respectively, Equation 22 & 23 are obtained.

$$\frac{\partial n}{\partial t} = \frac{1}{q}\Delta.Jn - Rn + Gn \tag{22}$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\Delta.Jp - Rp + Gp \tag{23}$$

3.2.2 Current-Density Equations: - The electron and hole current densities inside a semiconductor, $\boldsymbol{J_n} and\, \boldsymbol{J_p}$ are obtained by adding the current densities due to drift and diffusion.

$$J_N = qn\boldsymbol{\mu_n}\xi + qD_N\nabla_n \tag{24}$$

$$J_p = qn\boldsymbol{\mu_p}\xi + qD_p\nabla_p \tag{25}$$

3.2.3 Poisson's Equation: - The Poisson's equation (26) relates the divergence of the electric field to the space charge density, ρ.

$$\nabla.\xi = \frac{\rho}{\varepsilon_r\varepsilon_0} \tag{26}$$

In this equation ε_r is the semiconductor dielectric constant and ε_0 is the permittivity of the vacuum. The permittivity of the vacuum ε_0 = 8.854x10^{-14} F/cm and for c-Si ε_r = 11.7. Free electrons, holes and ionised dopant atoms are the main contributors to the charge density inside a semiconductor. It has been mentioned that impurities other than dopants and defects can be present in a semiconductor and act as charge capture centres. However, the concentration of such imperfections is kept small in semiconductors used for solar cells. The space charge density is therefore sufficiently described by Eq. (27):

$$\rho = q\,(p+N_D^{+} - n - N_A^{-}) \tag{27}$$

3.2.4 Recombination losses: - Electron-hole pairs generated due to incident photons are termed as carriers. These generated carrier's needs to be separated before recombination and emission of energy.

This recombination is the major cause of the loss of photo-generated carriers and due to this overall efficiency of a solar cell is affected. In a solar cell, recombination takes place at different regions as like generation of carriers in different regions. The generated carriers near the depletion region are separated by the electric field of depletion region whereas generated carriers in a solar cell at bulk, front and far end has a less probability to get separated. So, generated carriers in these regions will again recombine with the emission of absorbed energy and they will not contribute in the photovoltaic process. Hence, to improve the efficiency of solar cell recombination of those carriers must be governed. In photovoltaic solar cell following recombination losses affected the device performance.

i. Bulk recombination loss

ii. Interface recombination loss

iii. Recombination at metal-semiconductor contacts.

Bulk recombination loss: If impurities are present in the semiconductor material, then these impurities create energy states, which acts as a trap for photon generated carriers. A model for trap assisted bulk recombination loss is given by Shockley read hall recombination which is illustrated with the help of Figure 2.23 [66].

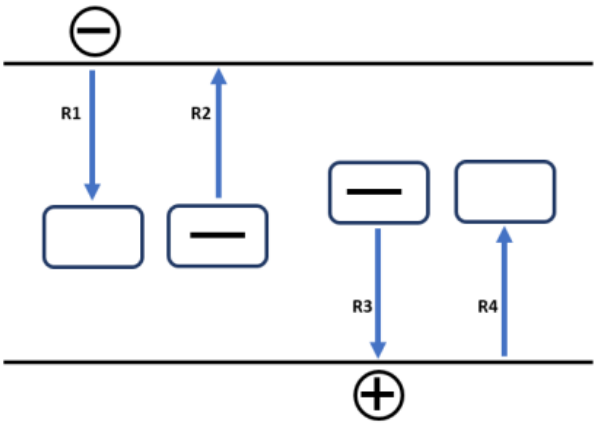

Figure 8: Generation of charge carriers by photon absorption
(Source:https://www.researchgate.net/publication/332736236_Modeling_of_High_Power_Conversion_Efficiency_Thin_Film_Solar_Cells)

Above figure shows the possible ways in which holes and electrons may recombine and

these processes are denoted by:

i. $R1$ a possible way with which electron will be capture at energy state Et.

ii. $R2$ emission of an electron from trap state.

iii. $R3$ capture of a hole.

iv. $R4$ emission of holes.

To find out the dependency of these processes on trap state, we will analyse these four processes individually.

For **R1** process: From Figure 2.23, trapping of an electron is depended upon the concentration of electron, defect density of state and probability of the empty state of these traps. Mathematically this is expressed in equation 2.27.

$$R1 = v_{th}\sigma_n n N_t (1 - f_t) \quad (28)$$

Where $v_{th}\sigma_n$ are proportionality constants, n is the concentration of electrons, N_t is density in trap states, and f_t is the probability of occupation of trap state for the electron. The expression for f_t is given in equation 2.28.

$$\text{ft} = \frac{1}{1 + \exp(\text{EtkT} - \text{Ef})} \quad (29)$$

E_t is energy of trap state and E_f is Fermi energy level.

For process **R2**: Electron is emitted into the conduction band and is expressed as the emission of an electron with the probability of occupation of trap state. The relation is given in equation 2.29.

$$R2 = e_n N_t f_t \quad (30)$$

Where en is emission of electron.

For process **R3** an **R4**: For hole capture and hole emission expression is given in equation 2.30 and 2.31.

$$R3 = v_{th}\sigma_n p N_t f_t \quad (31)$$

$$R4 = e_p(1 - f_t) \quad (32)$$

To find the emission rate for the electron, we assume that the capture of electron and emission of an electron from trap state are equal. So, relating $R1$ and $R2$ with each other, we can find the emission rate for an electron.

$$R1 = R2 \quad (33)$$

By putting value of $R1$ and $R2$ in equation 2.32 it will become

$$v_{th}(1 - f_t) = e_n N_t f_t$$

Further solving, rearranging for en and putting value for ft in equation 34 it will become as

$$\text{en} = \text{vth}\sigma\text{nn}\left(\frac{1}{\text{ft}} - 1\right) \quad (34)$$

$$en = v_{th}\sigma_n n\ exp(E_t - E_f)/\ kT \quad (35)$$

Where $n = (E_f - E_i)/\ kT$ and by putting the value of n we get

$$e_n = v_{th}(E_t - E_i)/kT \quad (36)$$

for ep the expression will be as given in equation 37.

$$ep = v_{th}\sigma_n n_i exp\ (\ ) \quad (37)$$

Now to derive the Shockley recombination model, we know that under equilibrium generation rate is equal to recombination rate.

$$G = U = R1 - R2 = R3 - R4 \quad (38)$$

So, solving it for equation 38 we will get equation 39 for total recombination.

$$U = Vth\sigma(\text{n}, \text{p})\text{Nt}\ \frac{\text{np} - \text{ni2}}{\text{n} + \text{p} + 2\cosh(\text{EtkT} - \text{Ei})} \quad (39)$$

From equation 39 it is evident that recombination is highly depending upon the density of defect states N_t, capture cross section for (electrons, holes) (n,) and concentration of (electrons, holes).

3.3 Introduction to SCAPS-1D: - Solar Cell Capacitance Simulator ($SCAPS$) program developed at the University of Gent, Belgium is used to simulate the photovoltaic devices. $SCAPS$ - $1D$ is the one-dimensional simulation program for the modeling of PV devices. Seven different semiconductor layers exclusive of back and front contacts are possible to take as input in $SCAPS$ - $1D$ software. $SCAPS$ - $1D$ tool is freely available for the photovoltaic research community and can be freely downloaded from its web link. It runs on a window operating system environment. This software is designed to simulate and helps us to analyse the J - V characteristics curve, ac characteristics (C - V and C - f), spectral response (QE) of a device, power conversion efficiency (PCE), fill factor (FF), short-circuit current (Jsc), open circuit voltage (Voc), energy bands of materials used in solar cell and concentration of different material used by solving the semiconductor basic equations [60,64,65].

3.3.1 Material Parameters:-For device modeling, input parameters or physical parameters are the fundamental requirements to solve the basic semiconductors equations. The physical parameters used in $SCAPS$ - $1D$ software for numerical analysis are layer thickness, electron-hole mobility, intrinsic

carrier concentration, electron affinity, band gap and doping density of absorber, buffer and window layers. Where Nv is the valence band effective density of state and Nc is the conduction band effective density of states in cm^{-3}. p is the hole concentration and n is electron concentration in cm-3, W is the thickness in µm. χ is the electron affinity in eV, Eg is the bandgap in eV,µe is the electron mobility in cm^2/Vs, µp is the hole mobility in cm2/Vs, All the simulations are conducted under 1.5AM solar radiation with the power density of 100 mW/cm^2 is used as the illuminating source. The device creation has two common objectives. First is the understanding and verification of real device behaviour and the second one is the simulation of a device for given physical parameters and predicting the outcomes for those parameters. A good device modeling is defined by the behavior of the reference device (s) was how much well simulated. For the creation of device modeling, physical or input parameters are collected form referenced device experimental data. $SCAPS$ offers a single simulation of J - V characteristics curve, ac characteristics $(C$ - V and C - $f)$ and spectral response (QE) and advance batch simulations by varying the input parameters. Predefined physical parameters such as carrier concentration densities and layer thickness are monitor and analyse with the help of batch simulations. J - V characteristics curve, band alignment diagram, spectral response and other functional parameters such as PCE, FF, Jsc and Voc are taken as output from *SCAPS-1D* software, which is very helpful for the fabrication of an efficient photovoltaic device. All measurements are calculated for illuminated or dark condition and as a function of temperature. Temperature-dependent parameters are the thermal velocity and effective density of states whereas band gap and mobility are temperature independent parameters.

Table 1: Physical parameters for numerical modelling

No.	Parameters	Abbreviation	Unit
1	Layer Thickness	W	Mm
2	Bandgap energy	E_g	Ev
3	Conduction band effective density of states	N_c	cm^{-3}
4	Valence band effective density of states	N_v	cm^{-3}
5	Dielectric permittivity	E_r	--
6	Electron affinity	X	eV
7	Hole mobility	M_p	cm^2/Vs
8	Electron mobility	M_e	cm^2/Vs
9	Electron doping concentration	N	cm^{-3}
10	Hole doping concentration	P	cm^{-3}
11	Absorption coefficient	A	cm^{-1}
12	Bulk defect concentration	N_T	cm^{-3}

13	Capture cross-section	Σ	cm^2
14	Defect energy level	E_T	eV
15	Metal work function	Φ_M	eV

3.3.2 SCAPS startup panel interface:- *SCAPS* - 1*D* simulator, start-up panel interface includes **(i)** *Section 1* is "Set problem" for the problem definition of the structure of a solar cell. Problem definition mainly having the details about the physical properties of different device layers. By clicking on the button "Set problem" another panel is open, where we define different layer physical properties.

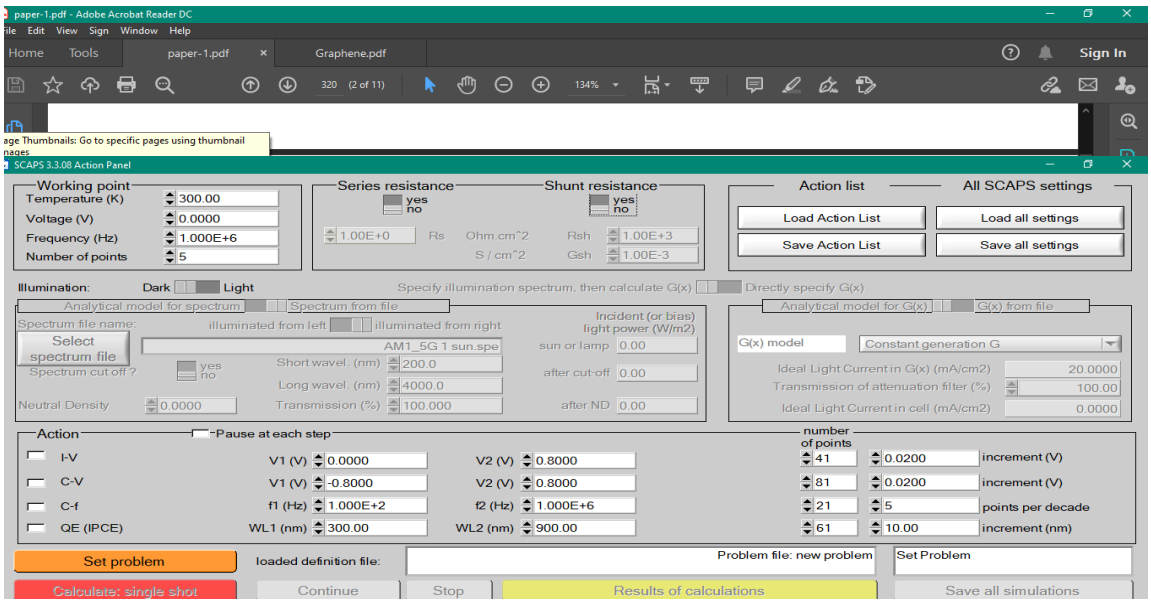

Figure 9: The SCAPS start-up panel

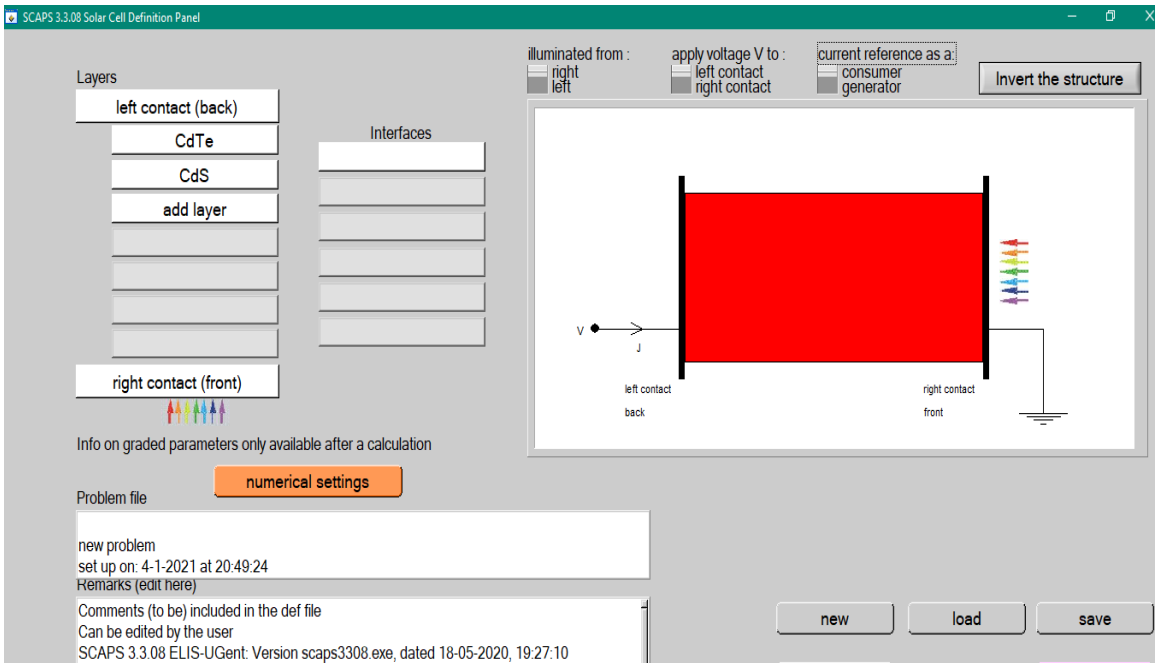

Figure 10: The SCAPS Interfacing panel

(ii) *Section 2* is "Action" pane for different measurements of simulations and reading scale settings. This section includes I - V characteristics scale settings and calibration, Quantum efficiency (QE) measurements, capacitance-voltage (C - V) measurements and capacitance frequency (C - f) measurements. Start and end values of argument and number of steps are adjusted if required (iii) Section 3 is "Illumination" for the selection of light and dark condition for simulation and spectrum standards. (iv) Section 4 is "Working point" for settings of working temperature values and addition of series or shunt resistances if required.

3.4 Fabrication technique of Thin film CdTe solar cell:- Thin film have a great impact on the modern era of technology. The crucial issue for all applications of thin films depends on their morphology and the stability. The morphology of the thin films strongly hinges on deposition techniques. Thin films can be deposited by the physical and chemical routes. Some advance techniques and principles of thin-film depositions are vacuum thermal evaporation technique, electron beam evaporation, pulsed-layer deposition, direct current/radio frequency magnetron sputtering.

3.4.1. Evaporation Technique: - Evaporation methods are considered as the common deposition of materials in the form of thin-layer films. The general mechanism of these methods is obtained by changing the phase of the material from solid phase to vapour phase and converting again to solid phase on the specific substrate. It takes place under vacuum or controlled atmospheric condition.

(i) Vacuum Thermal Evaporation Technique: - Thermal evaporation is a common method of physical vapour deposition (PVD). It is one of the simplest forms of PVD and typically uses a resistive heat source to evaporate a solid material in a vacuum environment to form a thin film. The material is heated in a high vacuum chamber until vapour pressure is produced. The evaporated material, or vapour stream, traverses the vacuum chamber with thermal energy and coats the substrate. This thin film deposition method is used most commonly for applications involving electrical contacts, by depositing metals like aluminium or silver.

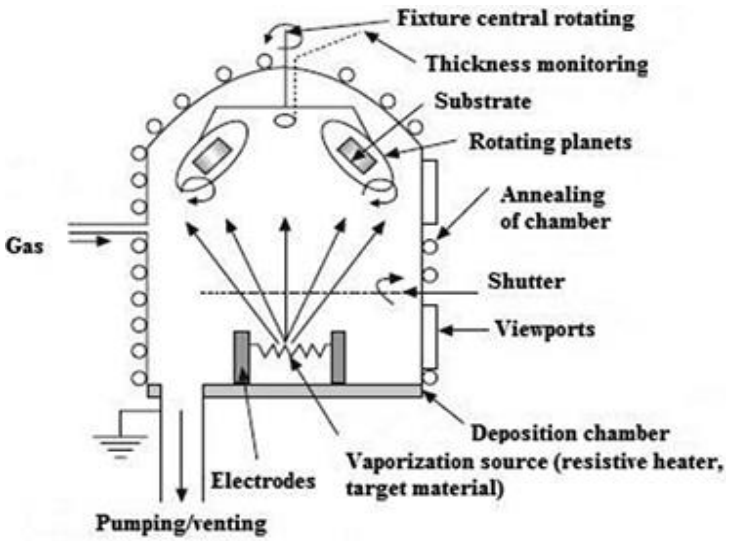

Figure 11: Schematic of thermal evaporation system with substrate holder.
(Source: https://cdn.intechopen.com/pdfs/52684.pdf)

(ii) Electron Beam Evaporation Technique:- E-Beam or Electron Beam Evaporation is a form of Physical Vapour Deposition in which the target material to be used as a coating is bombarded with an electron beam from a charged tungsten filament to evaporate and convert it to a gaseous state for deposition on the material to be coated. Taking place in a high vacuum chamber, these atoms or molecules in a vapour phase then precipitate and form a thin film coating on the substrate. E-Beam Evaporation, which is a Thermal Evaporation process, and Sputtering are the two most common types of Physical Vapour Deposition or PVD.

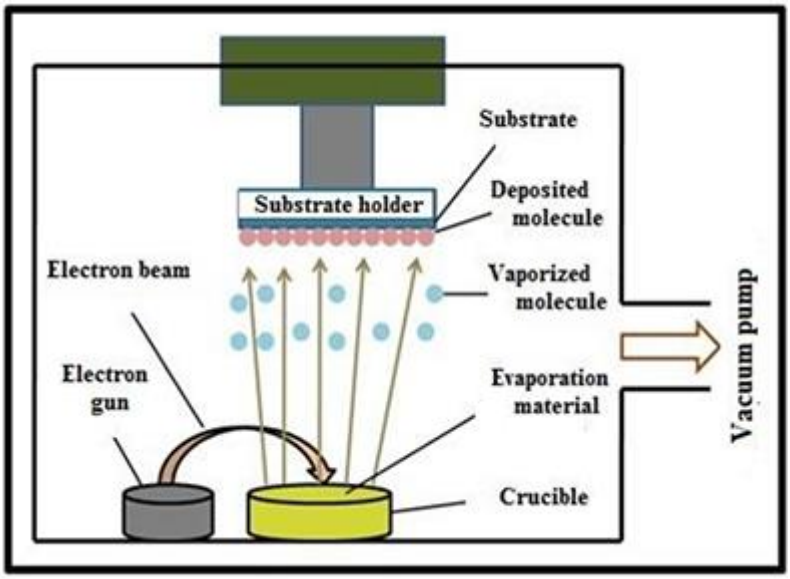

Figure 12: Schematic diagram of electron beam evaporation.
(Source: https://cdn.intechopen.com/pdfs/52684.pdf)

(iii)Laser Beam Evaporation Technique (pulsed-laser deposition):- Pulsed laser deposition (PLD) is a physical vapour deposition technique where a high power pulsed laser beam is focused to strike a target of the desired composition. Material is then vaporized and deposited as a thin film on a substrate facing the target. This process can occur in ultra-high vacuum or in the presence of a background gas, such as oxygen when depositing films of oxides

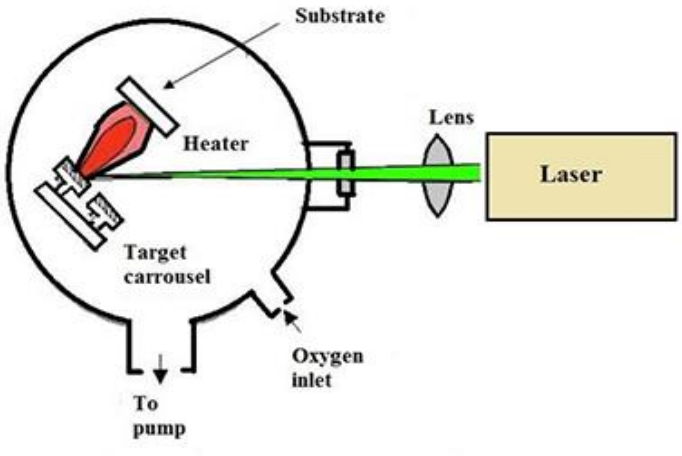

Figure 13: Schematic diagram of Pulse laser deposition
(Source: https://cdn.intechopen.com/pdfs/52684.pdf)

3.4.2. Sputtering Technique: - Sputtering technique is mostly used for depositing metal and oxide films by controlling the crystalline structure and surface roughness. The simple form of the sputtering system consists of an evacuated chamber containing metallic anode and cathode in order to obtain a glow discharge in the residual gas in the chamber. Also, an applied voltage in the order of several KeV with pressure more than 0.01 mbar is sufficient for film deposition. The sputtering process depends on the bombardment of the ions released from the discharge to the molecules in the cathode leading to the liberation of the molecules from the cathode with higher kinetic energy. The atomic weight of the bombarding ions should be nearly to that of the target material in order to maximize the momentum transfer. These molecules move in straight lines and strike on the anode or on the substrate to form a dense thin film. The process of sputtering has several advantages. High-melting point materials can be easily formed by sputtering. The deposited films have composition similar to the composition of the starting materials. Sputtering technique is available to use for ultrahigh vacuum applications. The sputtering sources are compatible with reactive gases such as oxygen.

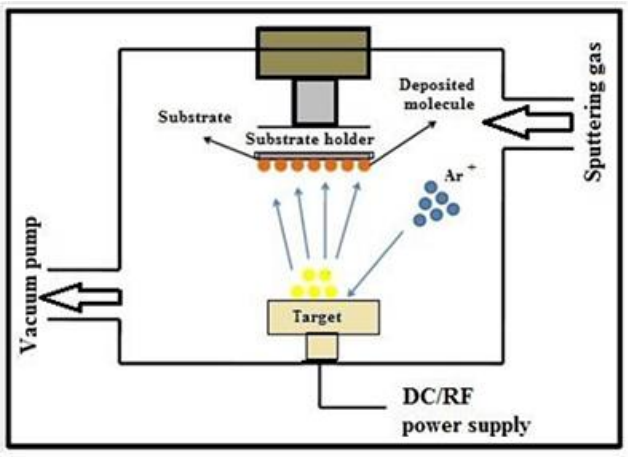

Figure 13: Schematic diagram of sputtering system.
(Source: https://cdn.intechopen.com/pdfs/52684.pdf)

4. Proposed research objectives

The key objectives of this research work are:

1. To improve the optoelectrical properties of thin-film CdTe and perovskite heterojunction solar cells in order to develop high-efficiency heterojunction solar cells
2. To optimize the absorber layer, employing a set of new techniques such as top- and back-contact texturing, plasmonic structures, and nanowires to enhance photon absorption.
3. To propose a new design structure for the efficiency enhancement of thin film solar cells by optimization of the charge selective layer in thin film heterojunction solar cells.
4. To explore different types of contact materials like oxide-based, lead-based, and alkaline-based, their contact properties, and interface defects for reduction of losses to improve performance.
5. To study the instability and degradation mechanisms in thin film CdTe, and perovskite heterojunction solar cells and develop mathematical models to predict the life cycle of the thin film heterojunction module.

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